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Modelling of substituents electronic and steric effects for effective analysis of organoelement and organophosphorus reactivity

Galkin V., Cherkasov A., Cherkasov R.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

For the effective analysis of organic and organoelement reactivity and the reaction mechanisms we have elaborated a simple enough models of steric and inductive substituents effects, which allow to calculate theorically the steric and inductive constants of any substituent at any reactive center. Both of these models possess of clear and comprehensible physical meaning, their correctness was confirmed by a good agreement of theorically calculated constants with well-known experimental steric and inductive scales. The wide possibilities of the suggested models for investigation of reaction mechanisms, organic and organoelement (organophosphorus, in particular) reactivity are discussed on the basis of different important organophosphorus reactions Pudovik, Abramov, Willyamson, Kabachnic-Fields reactions, acidic-basis equilibria, addition and complexation processes, etc.).